A MONTE CARLO STUDY OF THE ANISOTROPIC N=3 ASHKIN-TELLER MODEL

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Abstract

The phase diagram of an asymmetric N=3 Ashkin-Teller model is obtained by a numerical analysis which combines Monte Carlo renormalization group and reweighting techniques. Present results reveal several differences with those obtained by mean-field calculations and a Hamiltonian approach. In particular, we found Ising critical exponents along a line where Goldschmidt has located the Kosterlitz-Thouless multicritical point. On the other hand, we did find nonuniversal exponents along another transition line. Symmetry breaking in this case is very similar to the $N = 2$ case, since the symmetries associated to only two of the Ising variables are broken. However, for large values of the coupling constant ratio $X_W = W/K$, when the only broken symmetry is of a hidden variable, we detected first-order phase transitions giving evidence supporting the existence of a multicritical

point, as suggested by Goldschmidt, but in a different region of the phase diagram.

1 Introduction

A great deal of information about the N-color Ashkin-Teller model [1] (ATM) has been obtained in the past few years [2],[3], [4]. Several techniques, first applied to the particular case $N = 2$ (equivalent to a staggered eight vertex model) have been extended to the general case. One of them was the mapping of the statistical model onto a field theoretical one. After taking the time-continuous and scaling limits, Shankar [5] showed that the field theoretical counterpart of the isotropic N-color ATM is the Gross-Neveu model [6] (GN), extending in this way the mapping of the simple case ($N = 2$) to a Thirring model [7],[8] which in turn is equivalent to the quantum sine-Gordon equation [9]. Based on that equivalence he was able to prove that the ATM undergoes a first-order phase transition , whenever $N \geq 3$, similar to a result first obtained by Fradkin [10] in the limit $N \to \infty$. Mean-field calculations, Monte Carlo simulations [11] and $1/N$ expansions were also used to investigate the model. In particular we draw attention to [12], where Goldschmidt studied a modified version of the $N = 3$ ATM whose counterpart is an anisotropic Gross-Neveu model. Following Witten [13], he found the correspondence between his GN model and a supersymmetric sine-Gordon theory. The renormalization group flow equations were then used to argue in favor of the existence of a Kosterlitz-Thouless multicritical point [14] separating the first and second order transition lines. To compare his predictions with the expected phase diagram of the ATM he carried out a mean-field calculation similar to the one performed by Grest and Widom [11] to study the isotropic case.

The purpose of this paper is to investigate the anisotropic model studied by Goldschmidt by means of numerical simulations. The main conclusion of this paper is that our results rule out the existence of a multicritical point in the line where it was expected. Nevertheless, existence of a multicritical point cannot be ruled out at another line. These results have been obtained by employing a Monte Carlo renormalization group (MCRG) approach [15] improved by reweighting techniques [16],[17]. In the following section we describe the model as well as the results obtained by Goldschmidt. In section 3 we obtain the phase diagram and section 4 is devoted to the calculation of the critical exponents via MCRG. Finally in section 5 we discuss the results and comment implications and future work.

2 The model

The two-dimensional anisotropic $N = 3$ ATM considered by Goldschmidt consists of three Ising spin systems ($S^\alpha(\overrightarrow{r})$, $\alpha = 1, 2, 3$) coupled pairwise by four spin interactions of different strength. More precisely, he studied the Hamiltonian

$$-\beta H = \sum_{<\vec{r},\vec{r}'>} \sum_{\alpha=1}^{3} K S^\alpha(\vec{r}) S^\alpha(\vec{r}') + \sum_{<\vec{r},\vec{r}'>} \sum_{\alpha \neq \beta}^{3} U_{\alpha\beta} S^\alpha(\vec{r}) S^\beta(\vec{r}) S^\alpha(\vec{r}') S^\beta(\vec{r}') \quad (1)$$

where

$$U_{\alpha\beta} = \begin{pmatrix} 0 & w & u \\ w & 0 & u \\ u & u & 0 \end{pmatrix} \quad (2)$$

and the sum on $< \vec{r}, \vec{r}' >$ runs only over nearest neighbors. When $u = w$ we recover the symmetric N=3 ATM. In this case the model is equivalent [5] to the $N = 3$ Gross-Neveu model described by the Lagrangean

$$\mathcal{L} = (1/2) \sum_{i=1}^{3} \bar{\Psi}^i i \partial \Psi^i + g (\sum_{i=1}^{3} \bar{\Psi}^i \Psi^i)^2 \quad (3)$$

where ψ is a Majorana spinor, related to the spin operators (σ_i^α) associated to the classical variables (S^α) by the equations

$$\sqrt(2) \psi_1^\alpha(n) = \prod_{-\infty}^{n} \sigma_1^\alpha(m) \sigma_3^\alpha(n+1), \quad (4)$$

and

$$\sqrt(2) \psi_2^\alpha(n) = \prod_{-\infty}^{n-1} \sigma_1^\alpha(m) \sigma_2^\alpha(n). \quad (5)$$

In the more general case $(u \neq w)$, the model can also be expressed in a field theoretical language but the O(3) symmetry is explicitly broken. The equivalent Lagrangean now, is given by

$$L = (1/2)\sum_{i=1}^{3}\bar{\psi}^i i\partial\psi^i + g(\sum_{i=1}^{3}\bar{\psi}^i\psi^i)^2 + (\lambda - g)(\bar{\psi}^1\psi^1 + \bar{\psi}^2\psi^2)^2 \qquad (6)$$

where the parameters g and λ are functions of the four spin couplings u and w. In both cases the model can be mapped onto a supersymmetric (SUSY) sine-Gordon model, whose Lagrangean is

$$L = (i/4)\overline{D}\Phi D\Phi - (\mu/a\beta^2)\cos(\beta\Phi) \qquad (7)$$

where Φ is the superfield and μ and β are functions of g and λ. Based on the renormalization group flow equations for the coupling constants μ and $\delta = (\beta^2/4\pi) - 1$, which are characteristic of a Kosterlitz-Thouless [14] transition, Goldschmidt has advanced the existence of a KT point separating the continuous from the first-order transition line. To locate it he used a mean-field approach [11] previously used in the symmetric case.

The phase diagram obtained [12] in the subspace $u = 0.056$ is shown in Fig. 1. The relevant features of that diagram are: 1) the presence of first and second-order phase transitions separating the Baxter phase (I) and the paramagnetic (V) one; 2) first-order transition lines separating phase II from phases I and III; 3) symmetry breaking of two of three kind of spins in phase II and 4) the existence of a Kosterlitz-Thouless multicritical point at the end of the second-order transition line which separates phases I and V.

3 Phase Diagram

To investigate the consequences of O(3) explicit symmetry breaking of the $N = 3$ ATM we have performed Monte Carlo simulations combined with renormalization group and histogram techniques [18]. The phase diagram thus obtained is shown in Fig. 2. It summarizes the central results of this paper. Unlike that shown in Fig. 1 there is no first-order transition line separating phases I and V. In addition, in phase II, only the special family of spins (S^3) exhibits spontaneous symmetry breaking. The entire transition line **ABCD**, as well as the **HBI** one, belongs to the Ising-like universality class. The only nonuniversal transition line is the **GCJ** one. It separates phases I and II, where Goldschmidt found a first-order transition line, and phases V (paramagnetic) and VI (partially broken symmetry). While crossing from

V to VI, two classes of spins, S^1 and S^2, exhibit spontaneous symmetry breaking simultaneously. We now give the technical details of how the phase diagram was obtained.

We first located the transition lines using specific heat calculations (see Fig. 3). Data from the last temperature was taken into account to speed up thermalization. Histogram techniques were used to extend the results of a simulation around the neighborhood of the critical point, as well as to confirm, by the cumulant method [20], the existence, location and the order of the phase transition. This method, which in essence, uses the kurtosis of the energy probability distribution to distinguish between one and two-peaked distributions, and is very useful in determining the order of the transition, is discussed bellow. Figure 4 shows plots of the magnetization that were useful in determining whether a transition is ferromagnetic or antiferromagnetic. It can be seen that the first peak of Fig. 3 is associated with an antiferromagnetic transition, represented by open circles in Fig. 4. This transition corresponds to line **HBI** of the phase diagram in Fig. 2. The second peak is associated with a ferromagnetic transition (full squares in Fig. 4) and refer to line **GCJ** of the phase diagram. By this procedure the other lines of the diagram were constructed .

At this point, a discussion regarding the errors is opportune. There are two sources of errors: one of them has statistical nature. To calculate them is enough to perform a coarse grained calculation in which a long simulation is divided in, say 10 parts and the partial results are used for error estimation. For a lattice of linear dimension $L = 30$, the fourth order cumulant, described below, has errors of the order of 10^{-5} for $N = 10^7$ Monte Carlo steps (MCS) divided in 10 shorter simulations of 10^6 MCS each. Those errors decrease as $N^{-\frac{1}{2}}$ for a fixed value of L and as L increases, N should increase as L^2 in order to maintain the magnitude of the errors. The second source of errors is inherent to the histogram method. To minimize them it is a must to perform the simulations in the scaling region as suggested by the following arguments [19]. Let T be the simulated temperature where the energies E are stored in a histogram whose width is δE and $C(T)$ is the specific heat. Then

$$\delta E \propto [C(T)L^d]^{\frac{1}{2}}, \tag{8}$$

where L^d is the volume of the system. When the temperature is changed to $T + \Delta T$ the peak position of the histogram shifts by an amount proportional to $[C(T)L^d]\Delta T$. For reliable extrapolations the maximum value for ΔT_{max} occurs when the shift is equal to the width, i.e.,

$$\Delta T_{max} \propto [C(T)L^d]^{-\frac{1}{2}} \propto L^{-y_t}, \tag{9}$$

where y_t is the thermal critical exponent and $C(T)$ scales as $L^{\alpha * y_t}$ with $\alpha = 2 - d/y_t$. This would mean that calculations are less reliable as L increases and the extrapolation $L \to \infty$ would not be possible. On the other hand the shift between the real critical temperature and finite critical temperature estimates also decreases as L^{-y_T} and this result makes possible the extrapolations to higher values of L as long as the simulations are performed in the scaling region in order to keep valid the expressions above.

In what follows we discuss how to determine the order of the phase transitions. We use the peaks of the specific heat to locate the temperatures which will be used in the histogram techniques simulations. Consider the function V_L [20] obtained from the fourth cumulant of the probability distribution function of the energy E and given by

$$V_L = 1 - \frac{< E^4 >}{3 < E^2 >^2}. \tag{10}$$

The minimum value of V_L is a relevant quantity, since in the thermodynamic limit, for systems undergoing second order transitions, it is $2/3$, whereas a non trivial value ($\neq 2/3$) is the signature of a first order transition [20, 21]. The minima of V_L were estimated for several lattice dimensions L. An extrapolation, to simulate the thermodynamic limit $L \to \infty$ was made to obtain the order of the transition.

An example of the type of results obtained from these calculations is shown in Fig. 5, for a first order transition at $X_w = W/K = 2.0$. The extrapolated value for the cumulant gives 0.6626 and is very near $2/3$. The difference, however is significant as the errors are of order 10^{-4} and do not affect significantly the third decimal place in the extrapolated value. That value (e.g. third decimal place $2 \neq 6$) indicates a first order transition with very small latent heat. In order to obtain more evidence of the order of transitions, we analyzed the histograms $P_L(E)$ of the energy which should show two peaks. The distance between the peaks is the latent heat. As this value is rather small, the histograms exhibits a *plateau* , significantly different of the histograms associated with second order transitions, which clearly resemble a Gaussian form. Fig. 6 shows one histogram from a first order transition. We fitted the histogram with a symmetric mixture of two

Gaussians, centered respectively at E_1 and E_2, and used equation [22, 23]

$$V(L)_{min} = \frac{2}{3} - \frac{1}{12}\left(\frac{E_1}{E_2} - \frac{E_2}{E_1}\right)^2 + AL^{-d} \tag{11}$$

where A is a correction coefficient. For $d = 2$ and $A = -14.13$, obtained from the linear fit exhibited in Fig. 5, the equation above reproduces the four values of $V(L)_{min}$ from that figure within an error less than 10^{-4} (same order as the statistical errors). We conclude that we can use Eq. 11 for the minima of the cumulants and that the value 0.6626, the extrapolated value to infinite lattice size, indicates a first order transition. To confirm the existence of first-order transitions across line **GF** we used three different approaches to analyze the critical behavior along the line $X_W = 4$, where the first order character of the transition is more easyly detected. First, the two-point nearest neighbor correlation functions of a system of lattice size $L = 8$ and of another of size $L/2 = 4$ (see next section for renormalization details) were compared in Fig. 7 for different values of K. We observe that this behavior is completely different from that shown in Fig. 8, for the value $X_W = 0.8$, where the transition is clearly a second order one. In the Monte Carlo Renormalization Group (MCRG) approach the existence of a crossing or fixed point at the phase bounday indicates a second order transition, whereas its absence makes the case for a first order transition.

Next, we take the finite critical coupling estimates for several lattices, obtained when the magnetization is .5, to build Fig. 9 where we plot $K_c(L)$ against L^{-2}. A linear fit of those estimates confirms (R=0.9993) the validity of the relation

$$K_c(L) = K_c(1 - aL^{-2})$$

leading to the extrapolated value $K_c = 0.10632(3)$ for the critical coupling when $L \to \infty$. The exponent 2 which governs the approach of the estimates $K_c(L)$ to the actual value K_c indicates a first-order phase transition since the shift between the real critical temperature (inverse of coupling constant) and finite critical temperature estimates (see Eq. (9)) is known to decrease as L^{-y_T} (L^{-d}) in a second (first)-order transition [26]. Finally, we plotted the magnetization M (at the extrapolated K_c) against L, as shown in Fig. 10. The line presented in the log-log plot obeys the relation $M \propto L^y$ with $y = 1.95 \pm 0.05$, suggesting again that we are dealing with a first-order phase transition [27].

We also made a comparison with the $N = 3$ isotropic AT model studied by Grest and Widom [11]. They performed Monte Carlo simulations to determine the phase diagram. One of the effects of the breaking the symmetry between variables (S^1, S^2) and (S^3) is the appearance of the Ising-like line **ABCD** associated with the symmetry breaking of (S^3). Only phase I (a Baxter phase) has the same parameters ordered in both cases. In our diagram all the other phases have order parameters associated with variables (S^1, S^2) very different from that associated with (S^3) which does not happen in the isotropic case.

4 MCRG calculations

Finally, to calculate the associated critical exponents, we write the Hamiltonian at the n^{th} stage of renormalization as a linear combination of products of either spins of the same family or combinations of the three kinds (see Table 1).

We call the attention of the reader for the new meaning of S, now representing combinations of the classical spins S^α, which are explained in Table 1. As usual, we calculate the matrix $T_{\alpha\beta}$, associated to the linearized RG transformations, from the generalized specific heats

$$D_{\alpha\beta}^{(n)} = < S_\alpha^{(n)} S_\beta^{(n)} > - < S_\alpha^{(n)} >< S_\beta^{(n)} > \tag{12}$$

$$\widetilde{D}_{\alpha\beta}^{(n+1)} = < S_\alpha^{(n+1)} S_\beta^{(n)} > - < S_\alpha^{(n+1)} >< S_\beta^{(n)} > \tag{13}$$

and

$$T_{\alpha\beta}^{(n+1,n)} = \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}} = \left[D^{(n+1)} \right]_{\alpha\gamma}^{-1} \widetilde{D}_{\gamma\beta}^{(n+1)}. \tag{14}$$

For a blocking transformation with size b, this matrix has eigenvalues of the form b^{y_i}, y_h (resp. y_t) being the dominant eigenvalue of the odd (resp. even) sector. Table 2 shows the main eigenvalues at several critical points of the phase diagram. As we can see the values for the critical eigenvalues y_h and y_t, along the line **ABCD**, are very close to the Ising values 1.875 and 1.0. They do not depend on the value of the critical couplings $(K, Xw = W/K)$. The same occurs for lines **HBI** and **GE**. In this sense, the possibility of obtaining a Kosterlitz-Thouless multicritical point along the **ABCD** line is ruled out. The same is not true for the **GCJ** line. Critical exponents at that line show strong dependence on the coupling constants. In addition, we detected at that line the presence of a marginal operator in the renormalized Hamiltonian. This kind of operator, characterized by an eigenvalue equal to zero [24] (see last column of Table II - line **GCJ**), is able to change continuously the critical exponents [25]. Thus, we conclude that the transition along that line is nonuniversal. By taking into account the existence of first-order phase transitions, along line **FG**, for $X_W > 1$, necessary conditions for obtaining the multicritical point proposed by Goldschmidt could be fulfilled. However, note that the nature of the symmetries breakings associated to this transition is completely different from those described in [12].

5 Conclusions

We have used a combination of MCRG and reweighting techniques, as well as fourth order cumulant analysis to obtain the phase diagram and critical exponents for the two-dimensional anisotropic $N = 3$ Ashkin-Teller model. That model was proposed by Goldschmidt who succeeded in mapping it to a supersymmetric sine-Gordon (SUSY) theory. The phase diagram, as obtained within the mean-field approximation, exhibits second and first-order transition lines separating the Baxter and paramagnetic phases. At this line, the author has found a multicritical point of Kosterlitz-Thouless kind. Our MCRG calculations have indicated that there is no first-order transition line between the Baxter and paramagnetic phases. Thus, the possibility of finding a multicritical point along the line **ABCD** is ruled out. In addition, we obtained a symmetry breaking in the phase II which is completely different from that found by Goldschmidt. We also calculated the critical exponents along the continuous transition lines and observed that only the **GCJ** line is nonuniversal. As we showed that this line also presents first-order transitions, for values of X_W greater than 1, we conclude that the multicritical point, if it exists at all, should lie on the **FGCJ** line. However, the symmetries of the phases VI and VII are only partially broken. Thus, we have no evidence of the existence of a Kosterlitz-Thouless-like multicritical point along this line.

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Table Captions

Table 1. Notation for the operators used in the MCRG analysis. We use (σ, μ, τ) to represent the spin variables (S^1, S^2, S^3).

Table 2. Estimates for odd (even) $y_h(y_t)$ eigenvalues associated with the transition lines. The values were obtained after the 2^{nd} step of the renormalization process for lattice 32x32 including all odd (even) operators. Numbers between parenthesis mean the values of the statistical errors, calculated from group of ten partial runs of 10^5Monte Carlo steps.

Table 1

Even sector	
$S_2 = \sum_{nn}(\sigma_i\sigma_j + \mu_i\mu_j + \tau_i\tau_j)$	$S_8 = \sum_{nnn}(\sigma_i\sigma_j + \mu_i\mu_j + \tau_i\tau_j)$
$S_4 = \sum_{nn}(\sigma_i\sigma_j\mu_i\mu_j)$	$S_{10} = \sum_{nnn}(\sigma_i\sigma_j\mu_i\mu_j)$
$S_6 = \sum_{nn}(\sigma_i\sigma_j\tau_i\tau_j + \mu_i\mu_j\tau_i\tau_j)$	$S_{12} = \sum_{nnn}(\sigma_i\sigma_j\tau_i\tau_j + \mu_i\mu_j\tau_i\tau_j)$

Odd sector
$S_1 = \sum_i(\sigma_i + \mu_i + \tau_j)$
$S_3 = \sum_{nn}(\sigma_i\mu_j)$

Table 2

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Line ABCD			
K	X_w	y_t	y_h
0.40	-1.0	0.97(2)	1.869(7)
0.34	0.60	0.98(3)	1.876(6)

Line HBI			
K	X_w	y_t	y_h
0.33	-1.7	0.92(5)	1.852(8)
0.51	-1.38	0.93(4)	1.862(9)

Line GE			
K	X_w	y_t	y_h
0.22	2.0	0.93(7)	1.848(9)
0.20	4.0	0.96(3)	1.876(6)

Line GCJ				
K	X_w	y_t	y_h	y_m
0.50	-0.29	0.83(5)	1.875(7)	0.08(2)
0.40	-0.02	1.12(6)	1.866(6)	-0.07(2)

Figure Captions

- Fig. 1. Phase diagram of the N=3 Ashkin-Teller model obtained within the mean-field approximation. The coupling u was fixed at the value 0.056. In the Baxter phase (I) all S^α and their products $S^\alpha S^\beta$ order. In phase II, only S^1, S^2 (or

  S^2 and S^3) and their product order. Phase V is the paramagnetic one. In phase IV only (S^1S^2) order antiferromagnetically whereas in phase III S^3 (ferro) and the product S^1S^2 (antiferro) are ordered. The Kosterlitz-Thouless multicritical point (MCP), located at the point $X_W =-0.2$, K=0.25, is also shown.

- Fig. 2. Phase diagram of the N = 3 Ashkin-Teller model obtained from Monte Carlo simulations. In phase I, all $\langle S^\alpha \rangle$ and $\left\langle S^\alpha S^\beta \right\rangle$ order. Phase II exhibits only ordering of the special class of spins S^3. Phase V is the paramagnetic one whereas phase IV presents antiferromagnetic order of the variable (S^1S^2). The phase transition along the entire line ABCD is continuous as well as the transition line which separates phases I and II. In phase VI, $S^1$and S^2 order but in phase VII only the product (S^1S^2) is ordered.

- Fig. 3. Plot of the specific heat as a function of X_W for K =0.5 (Same range as in Fig. 4).

- Fig. 4. Plots of magnetization for the spin variable (S^1S^2). Open circles represent the sum of (S^1S^2) for alternate sites whereas full squares contains the sum of (S^1S^2) for all sites.

- Fig. 5. Finite size scaling of the cumulant: linear fit of the minima of the

  fourth-order energy Binder´s cumulant versus L^{-2}. Error bars are of the size of the symbols.

- Fig. 6. Mixture of Gaussians fitting of the histogram for the energy E calculated with the variable (S^1S^2) . Simulations were done at the point X_W =2.0 and K_c =0.185 for a lattice size L =80.

- Fig. 7. Two-point correlation function of the product S^1S^2 for lattices of size $L = 8$ and 4 and $X_W = 4.0$

- Fig. 8 Two-point correlation function of the product S^1S^2 for lattices of size $L = 16$ and 4 and $X_W = 0.8$

- Fig. 9. Critical coupling estimates plotted against the inverse of the squared lattice size (L^{-2}). Error bars are of the size of the symbols. The linear fit $K_c(L) = K_c(1 - aL^{-2})$ confirms the order of the phase transition (first) and leads to the value $0.10632(3)$ for the critical coupling K_c, when $X_W = 4.0$.

- Fig. 10. Magnetization at the true critical coupling $K_c = 0.1063$ against the lattice size L in a log-log plot. The angular coefficient results 1.95 ± 0.05 corroborating the first-order character of the phase transition when $X_W = 4.0$.